Electronic Structure of Icosahedral AlPdMn

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Quasicrystals are a new class of materials with unexpected symmetry properties and a potential for applications in a wide range of fields [1]. The electronic structure of icosahedral quasicrystals is of great current interest, since in view of the unusual symmetry properties of these materials, conventional notions on electronic structure need to be adapted in order to provide a meaningful description of their properties. Among the striking features of quasicrystals are their high electrical resistivity and the low electronic contribution to the specific heat, compared to those of their metallic constituents. These features, and the specific heat finding in particular, still await an explanation in terms of the electronic structure of these materials. Here we report on a core and valence level photoemission study of icosahedral AlPdMn in order to assign regions of the valence band to the different atomic constituents, and to shed light on the atomic coordination in AlPdMn. Spectra were recorded from cleaved as well as sputter-annealed surfaces of surfaces with five-fold symmetry. A comparison of data from these different preparation methods can be used in order to investigate the possible influence of deviations from stoichiometry induced by sputter-annealing.

Figure 1 shows the core level spectrum of i-AlPdMn recorded at a photon energy of 400 eV, which shows the intense Al 2p and Pd 3d core levels, as well as a strong peak in the valence band region (also shown in the inset) which is ascribed contributions from the Pd 4d level. The satellite structure on the core level peaks, particularly prominent on the Al 2p, is due to plasmon losses.The atomic arrangement of the quasicrystal constituents is still a subject of intense research effort. We have therefore recorded the polar and azimuthal intensity variation of the strong core level lines. These patterns, which demonstrate that our quasicrystal surfaces exhibit good quasicrystalline order, are shown for the Al 2p and Pd 3d peaks in Figure 2. The left diagram shows the raw data of the Pd 4d peak, recorded over a polar angle range of about 250 degrees and an azimuthal range of 45 degrees. Even in the raw data the fivefold symmetry of the intensity distribution is clearly visible. The structures gain contrast when subjected to a smooth background subtraction and symmetrization procedure, as shown for both the Pd 3d and Al 2p levels in the center and on the right-hand side. These patterns, which arise from photoelectron diffraction, are currently being interpreted through multiple scattering diffraction calculations which are expected to yield information on the structure of the so-called pseudo-Mackay clusters which are thought to be the basic building blocks of quasicrystals, as suggested from recent scanning tunneling microscopy experiments [2], for example.

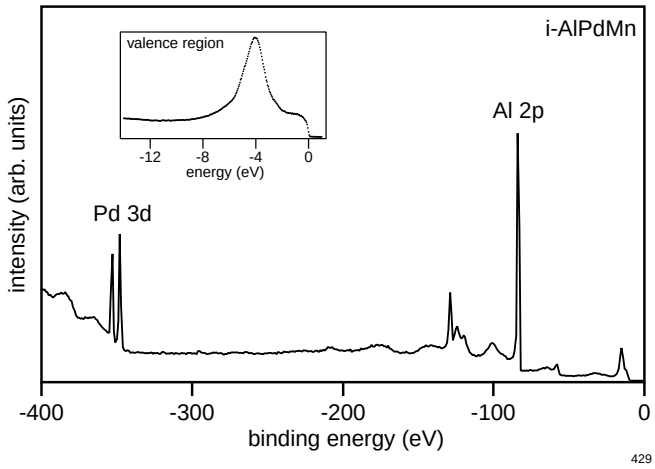

Figure 1: Core level spectrum of i-AlPdMn, displaying the intense Al 2p and Pd 3d lines. Inset: region of the valence band.

Spectra form the valence region of i-AlPdMn exhibit broad structure from which an assignment in terms of different atomic contibutions is not straightforward. The peak at about 4 eV below the Fermi level EF can be assigned to Pd 4d states because of its cross section upon photon energy variation, on account of the loss in intensity due to the Cooper minimum. The region of the valence band near EF can be attributed to Mn *s* states, from resonant photoemission experiments at the Mn 2p edge [3].

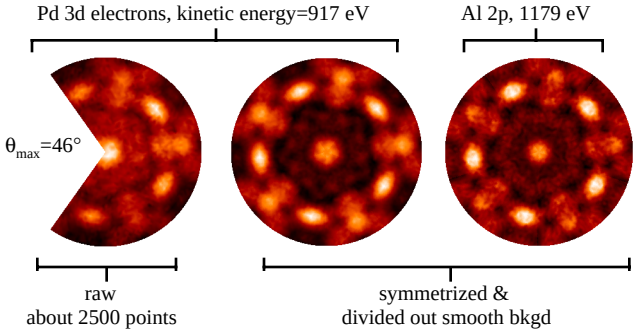

Figure 2: Angular variation of Pd 3d and Al 2p core level peak intensities, measured over a range of 250 ° polar and 45° azimuthal emission. The raw data (left) were subjected to a smooth background subtraction and symmetrization to yield the patterns in the center and on the right-hand side.

Many discussions of structure-induced features in the electronic spectra of quasicrystals are based on the concept of Brillouin zones, generalized in a vague way to quasicrystals. This generalization may actually be based on firm ground, by considering that the six-dimensional hypercubic lattice corresponds to a six-dimensional reciprocal lattice, in which the Brillouin zone may be defined in the usual way, being bounded by the planes bisecting the Q vectors that belong to the star of equivalent reciprocal lattice vectors. The special points in 6D reciprocal space can then be projected onto 3D reciprocal space to define quasiperiodically distributed special points. While the special points in this projection are dense everywhere, they are weighted by a generalized structure factor, and a quasi-Brillouin zone may be defined in terms of the strongest zone center and zone boundary special points[4]. The emission intensity as a function of angle from different regions of the valence band can give information on the symmetry of the states involved. This information has so far been lacking in conventional angle-resolved photoemission from quasicrystalline surfaces, since the features are rather broad and shifts upon variation of the parallel or normal component of the wave vector are difficult to detect. Thus, angular patterns from several regions of the valence band were recorded in a similar fashion to the ones shown in Figure 2. These also exhibit a marked angular pattern of fivefold symmetry, suggesting that the symmetry of the quasicrystal building blocks is indeed reflected in the valence states.

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